Defining Excellence - Modeling, Simulation and Visualization

High-Performance Computing (Supercomputing) - Numerical Simulation of Physical Problems

Modeling, scaling, artificial intelligence and visualization are tools scientists and engineers use to understand, shape and control the physical world. All are dependent on computers. The bigger the problem you want to solve, the larger the computer you need. But how big is big? How large is large?

According to Eric Greenwade, group leader of the Numerical Simulation Laboratory, large is a relative idea. "Large means different things to different people. I'll define large data sets (problems) as those we can barely handle."

His definition is based on what he calls 'a pain threshold.' People are willing to wait a certain amount of time for an answer or response. A Web surfer may be willing to wait a second or two for a browser to respond. Scientists running large-scale simulations might be willing to wait three weeks, months or years for an answer. It's a Catch-22 process. If you increase the amount of the hardware to speed the process, scientists will increase the size of the problem.

So while Greenwade leads some of the most advanced visualization and modeling efforts being conducted at the Laboratory, he makes his greatest impact with supercomputing.

David and Goliath

Say supercomputing and the mind's eye sees antiseptic rooms of giant, humming machines, served by white-coated scientists and programmers. Greenwade has these kinds of supercomputers; busy processing 50 gigabytes per second in air-conditioned, filtered rooms. But he also has supercomputers of the more mundane type - a gaggle of PCs, called cluster computing.

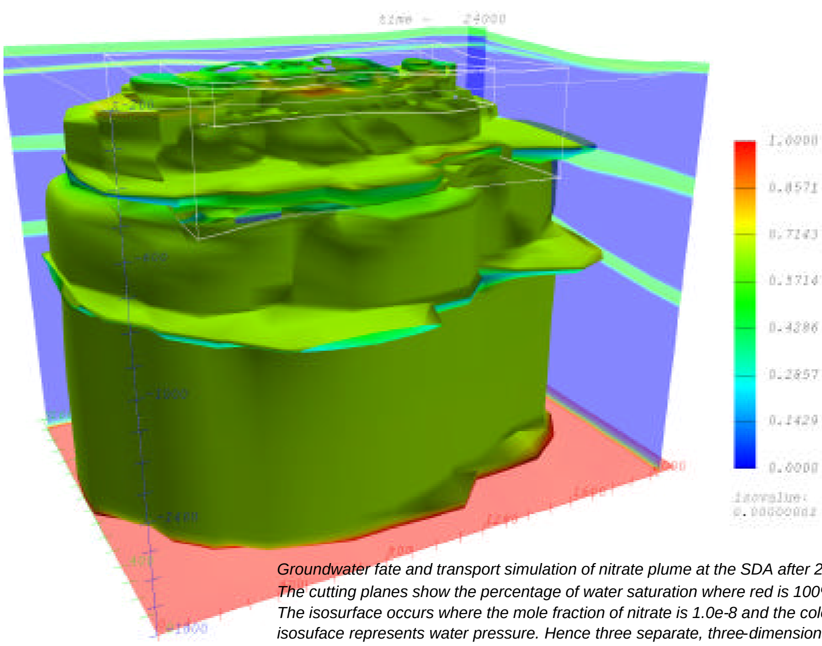
"It's more ying/yang than David and Goliath," said Greenwade, speaking of the relationship between clusters and symmetric multi processors (SMPs), the classic supercomputer. "It's not adversarial, but complementary." Clusters, although vastly cheaper than even the most bargain-basement supercomputer, require much more of an investment in time. Computer engineers need to know the details of the hardware, networks, operating system, applications and simulation code before they can begin to draw the computing power from the linked systems. SMPs handle all that automatically. But at $1.5 million for an SMP versus less than $100,000 for a cluster, it's a worthwhile learning curve.

Eric Greenwade stands with one of the newest multi-processors, also known as a classic supercomputer. The Numerical Simulation Laboratory has a number of high performance computer platforms available for use by INEEL scientists and collaborators.

Greenwade runs about half of the mathematical problems on clusters but he says only 10 percent of them run really well. He is focusing on how to make them run better. For the last three summers he has mentored talented computer science students in Beowolf-class cluster computing. He sees the future of scientific computing in understanding the true capabilities of clusters. "All the money in the world won't buy the supercomputing power we will need," says Greenwade.

The Big Picture - Jpeg

Some of the most valuable contributions Greenwade makes to the INEEL are not even done at the INEEL. Greenwade serves as official U.S. representative to the International ISO JPEG and MPEG Working Groups and is one of the authors of JPEG-2000's Annexes E, F and G. JPEG-2000 is intended to create the state-of-the-art compression for the next 10 years. While the novice computer user recognized .jpg as a format for photos sent over the Web, Greenwade explains its real purpose and value.



Groundwater fate and transport simulation of nitrate plume at the SDA after 24000 days. The cutting planes show the percentage of water saturation where red is 100% saturated. The isosurface occurs where the mole fraction of nitrate is 1.0e-8 and the color on the isosuface represents water pressure. Hence three separate, three-dimensional variables are being simultaneously displayed.

"In high-performance computing and particularly in visualization, we end up with very, very large amounts of data. That data needs to be processed efficiently and it needs to be moved around."

The concept of data compression is easily understood with the example of a photograph, scanned and e-mailed. During the wildfires last summer, a spectacular photograph of cow elk was taken by a firefighter and mailed around the world. The photo may comprise 1 or 2 megabytes of raw information. If you compressed that image to one-tenth, one-twentieth or one-hundredth of its original size, you could ship it faster, more frequently and with less impact to the infrastructure.

Some of the same techniques that are used to transmit data effectively via compression also help to process data effectively. Greenwade and the JPEG Working Group set the standards for the next generation of hardware, promoting the types of features that will support scientific work.

The standards body includes representatives from the hardware developers - Adobe, Sony, Kodak, Ricoh, Sharp, Cannon, etc. Greenwade's participation gives the INEEL a keen competitive edge. "We often know at least two years in advance what these capabilities are going to be and what the rest of the community is moving towards."

Wavelets of the Future

The new compression schemes offer other significant advantages to researchers over the old Fournier-Transform-based techniques in that they are hierarchical. For example, analysts looking at contaminant transport data can set up the representation so that data they are most interested in comes first. The analyst can then very, very quickly scan through the remainder. The compression scheme can be tuned to be sensitive to the data researchers are interested in because the important characteristics have been set up to represent the higher order of the coefficient.

The hierarchical approach is a tremendous advantage when the output is known and no disadvantage if it is unknown. These techniques are based on wavelets that focus on sharp changes. Humans see objects by edges and hear by changes in pitch. These sharp changes, non-differentiable jumps in data, are well-represented by wavelets and they do it at the first part of the file.

Greenwade is putting together all of these aspects - visualization, high-performance computing, data compression and transmission - into what he calls an interactive, collaborative environment.

Researchers collaborating on projects today often don't sit in side-by-side cubicles or even side-by-side laboratories. INEEL researchers work with other Department of Energy (DOE) laboratories, regional and national universities, and more and more frequently, scientists from around the world.

Greenwade's group is developing a system where colleagues can share images and test results while still retaining ownership of sensitive data. In real time, they can examine models, change parameters and discuss consequences as if they were sitting around the same workstation. Their first test of the system is scheduled for summer when they will be implementing a test version to visualize subsurface science data.

"This will be a tremendous tool for stakeholders," says Greenwade, who presented an invited paper on the concept in Tokyo this last April. "People are hesitant to accept everything at face value. They want to ask the question, 'Have you looked at this from a different perspective?' This type of tool can send the science right into the conference rooms."

Greenwade travels constantly; presenting invited papers, presiding over technical conferences and helping establish the next generation of standards. In Idaho, he leads his group in the creation of otherworldly visualization models grounded in the most fundamental science. In his spare time, he mentors new talent and explains computer games to children on PBS. And with each one of these activities, the INEEL benefits.

Greenwade sees the future of scientific computing in understanding and developing the true capabilities of clusters.

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Modeling - A mathematical or physical system, obeying certain specified conditions, whose behavior is used to understand a physical, biological or social system to which it is analogous in some way.

Forms of modeling vary almost as much as the types of projects that employ them. Physical system modeling mirrors a process; geometric solid modeling portrays an object.
Lyle Roybal has used many types of modeling at the INEEL and for other organizations, but some of his most dramatic projects used 3D model mock-ups. Roybal has modeled reactors, missiles, satellites and jets. At first glance, the model appears to be a photograph, but on closer examination the viewer sees the angles, planes and shapes of a computer mock-up. What the viewer does not see is that these models are truly multidimensional; beneath the skin lie vital components necessary for the object's performance.
The models are used to predict behavior. Reactor modeling is used to predict failure. Other models, such as those for weapons, predict success. Both offer a safer alternative to untested performance. From the information provided by the model comes the code that runs, guides and rules the object.

Not all modeling is as visually exciting as the geometric solid modeling. Sometimes modeling just results in better, safer and quicker ways of doing business.

Employees at Fernald Environmental Management Project (FEMP) in Ohio are using sodium iodide and germanium spectrometers to measure contamination. The instrument measures counts per second. Physicists at FEMP have developed models to turn these counts per second into isotopical concentrations. Roybal is implementing these models through algorithms with results available on a real-time basis. The process has valuable applications at INEEL and around the DOE complex.

Where the old process took four to five days for contamination results, radiation physicists and technicians now obtain that same information in real time. Instead of sending 100 or more samples to a lab for expensive and time-consuming analysis, the technicians can target appropriate areas and select a handful of more meaningful sample locations.

This technology is currently being used at the Idaho Nuclear Technology and Engineering Center (INTEC) to aid in a decontamination and decommissioning project.

Models, such as this 3D aircraft created by Lyle Roybal, are used to predict behavior and offer a safer alternative to untested performance.

In spite of his important contributions to environmental management, Roybal is probably best known at the INEEL for his work with National Security technologies. The Rapid Geophysical Surveyor and the Concealed Weapons Detection system are highly successful and nationally known. Both the RGS and the CWD have spun out to commercial enterprises and Roybal holds a patent on the weapons detection system.

The RGS is the primary survey tool for Idaho Falls small business Sage Earth Sciences and has been marketed nationally and internationally. Recently, an RGS system was included in the Transportable Munitions Assessment System sent to Greece to help with the discovery and destruction of obsolete weapons.

The Concealed Weapons Detector received national attention when it was installed in Bannock County Courthouse. Although these two inventions appear outwardly distinct, Roybal points out the similarities. “They both basically use the same sensor technology. With the Surveyor, the sensors move over the target. With the Weapons Detector, the target - people - move through the sensors.”

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Computer Science and National Security

Computer science may not at first glance appear to be a national security component. But the DOE recognizes that advanced computing lies at the heart of all technological advancement. A look at the DOE Headquarters National Security Web site confirms this view. Right there with categories of Security, Emergency Response, and Nonproliferation is Computing. And right there is modeling, simulation and visualization.

“National security has been the driving force in many of our country’s computational and communication advances," says Jane Gibson, manager of Advanced Information & Communication Systems and the Modeling, Simulation and Visualization group. In the 1960s, the Defense Advanced Research Projects Agency funded the creation of the Internet to ensure communications survivability.

Our nation’s security mission has historically required the fastest computers available. For example, DOE sponsors the Accelerated Strategic Computing Initiative, which uses terascale computers to simulate nuclear tests instead of conducting them. INEEL, for the first time in a long,

long time, is in the position of joining the top 500 club in high-performance computing with its recent acquisition of shared memory computers and improved connectivity to the research world.

In Intel's case, subsurface science is the driving force for our first major infrastructure improvements, and all other INEEL institutional plan initiatives have joined forces to leverage these investments to benefit all through the recent adoption of a company wide initiative, Advanced Computing and Collaboration Initiative."

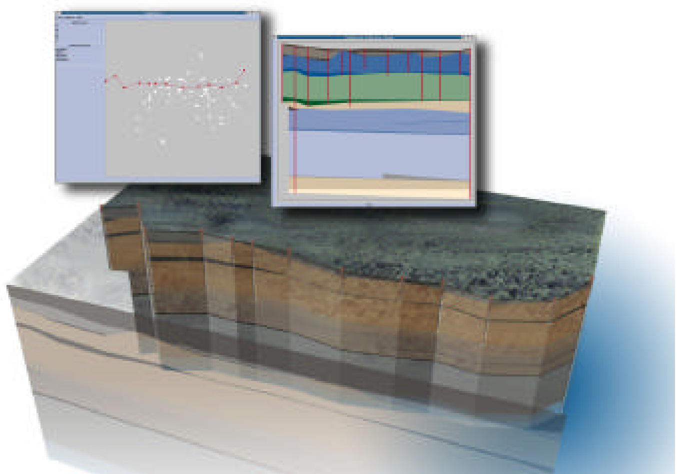
Gibson says the capabilities of the INEEL's National Security Modeling, Simulation and Visualization are superior. The reputation of key members is world-class and their research and development renowned. They define excellence.

Take a virtual tour of these capabilities through these brief descriptions of some of the organization's projects.

Simulation - The development and use of computer models for the study of actual or postulated dynamic systems.

Wells and boreholes dot the INEEL landscape like spots on a leopard's hide. Hundreds pierce the thin skin of the high-desert soil, auguring through layers of sediment and basalt. The depths range from the shallow vadose or geotechnical wells at less than 100 feet to the deep geological investigation boreholes sunk nearly 5000 feet into the subsurface.

In addition to performing the task they were drilled to do - supplying water or monitoring the environment - the wells tell the story of the earth beneath them. The wells reveal what rock types, at what depths lay in their path downward. Until recently, this information was more isolated, difficult and time-consuming to combine. But no longer. Steve Woolsey has developed a subsurface lithographic model that easily 'connects the dots' of the individual wells, offering a simulated view of the underworld.



Existing wells now yield a simulated view of the underworld thanks to a program developed by INEEL's Steve Woolsey. The program "connects the dots" of individual well data and offers WAG 7 researchers subsurface views typically seen only at road cuts. The sample program output shown on the computer screens at top is interpreted in the artist's rendering at bottom.

Woolsey's program peels back the skin of the Site and shows subsurface views of the INEEL typically seen only at road cuts or within open mines. Developed for Waste Area Group (WAG) 7 at the Radioactive Waste Management Complex, INEEL scientists researching the migration of contaminants through the labyrinth of rock, soil and water now have another tool.

The program started with a database containing the facts on each well - the types of soil and rock it drilled through and depths of each stratum. The database can be queried for each well. Woolsey added a 'rule set' developed by Steve Anderson, a geologist with the United States Geological Survey. The 'rule set' suggested logical guidelines for interpreting geological connections between two wells.

On a computer screen, INEEL wells are displayed on a map, and with a click of a mouse, Woolsey selects wells and connects them in a line. Using complex algorithms, the program interprets the individual well data and displays a view that Woolsey says, 'looks like the side of a mountain where an earthquake fault has risen and revealed the layers of earth." WAG 7 researchers can now visualize the surface beneath the INEEL and its complex layering of rock.

Woolsey's next step will be tying in the code for associate James Galbraith's visualization work with contaminant data. While developed specifically to address WAG 7 concerns, the program will be evaluated for site-wide use.

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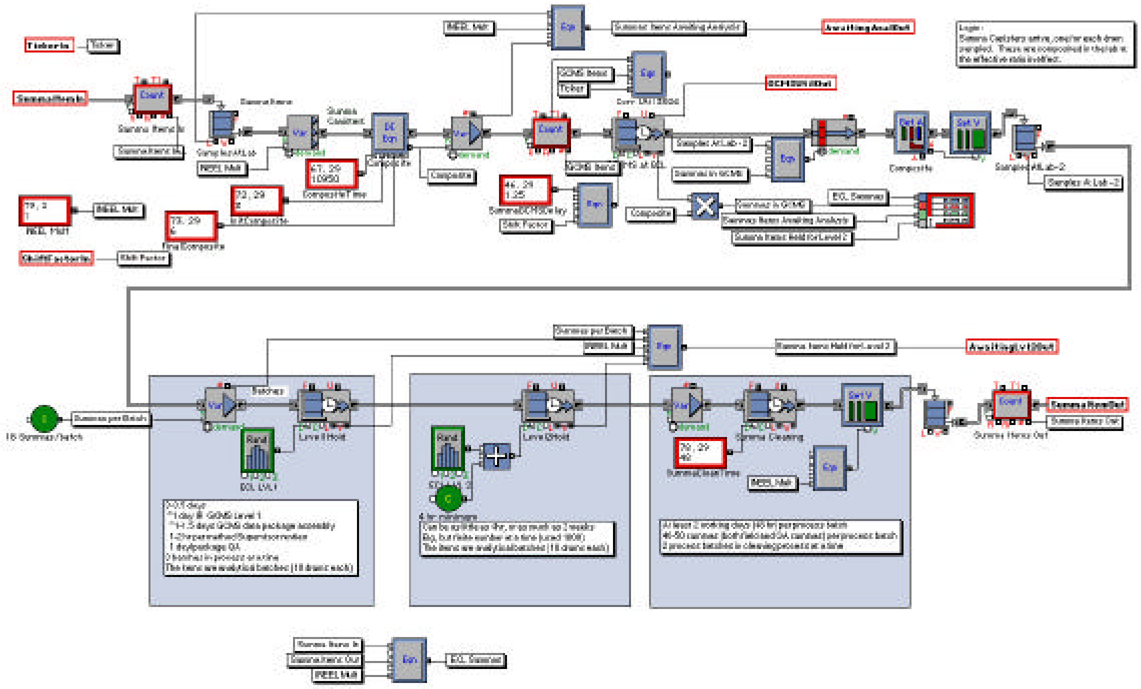

The INEEL TRU Waste System Model mirrors the actual process, step-by-step, decision point-by-decision point. It will help streamline processes such as the headgas sampling pictured above.

The INEEL committed to removing 3,100 cubic meters of transuranic waste from Idaho by December 31, 2002. To accomplish this, over 24,000 contact-handled 55-gallon drums will be examined at the Stored Waste Examination Pilot Plant to yield the 15,000 shippable drums. All of the drums undergo various processes including real-time radiography, gamma-ray spectrometry, venting, and headspace gas sampling before loading and shipping. Selected drums will also go through intrusive examination and sampling.

An onerous task at best, delays in opening the Waste Isolation Pilot Plant and changes to the waste acceptance criteria compressed the INEEL's performance time down to 27 months.

To ramp up for this massive production effort, the existing process had to undergo changes - but what changes? The right changes could increase productivity; the wrong ones could cause unacceptable delays.

That's where Dave Van Haaften came in. Van Haaften and Modeling, Simulation and Visualization supervisor Cathy Barnard created a system model of the complete INEEL TRU

waste project.

Based on a national model they developed for the Carlsbad Field Office, the INEEL TRU Waste System Model mirrors the actual process, step-by-step, decision point-by-decision point. The model was developed in Extend, a commercial discrete event simulation software package. The INEEL model simulates events that happen when items - in this case drums - move through the process.

Built into the system are the time delays - how long each operation delays a drum at any given point in the process. The delay data was developed from design files, project manager input and interviews with operators. The model shows the bottlenecks in the process.

The purpose of the model was to guide and validate planning and it has done that, demonstrating the need for additional capacity in several areas including real-time radiography. As a result, the first rental RTR began operating in April. A second 7 x 12 shift was based, in part, on the model's results.

Industrial manufacturers have long depended on discrete event models; 3100m^3 is one of the first 'production' projects on Site to develop one. The ability to view different scenarios before implementation of process changes has proven to be invaluable.

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Scaling - Expressing the terms in an equation of motion in powers of nondimensional quantities (such as a Reynolds number), so that terms of significant magnitude under conditions specified in the problem can be identified, and terms of insignificant magnitude can be dropped.

The INEEL has long been a center of excellence for use of scaling in research and development. And no better example exists than the Semiscale facility, constructed at the Water Reactor Research Test Facility in the early '70s. Roughly 1/1700th the size of a power reactor, this scaled-down version was built to help understand what happens in a massive loss of coolant accident (LOCA).

Tom Larson, engineer and science fellow, explained the concepts of scaling, Semiscale experiments, and some of the results. "Scaling culminates with the art of building a small system representing a larger system so that the first order of effects are preserved and the lower order effects are maintained as much as possible." Different size reactors, pipes and systems do not respond exactly the same; the art is recognizing the distortions and their effects.

"We were tasked to show if (power) plants could survive the worst case accidents. We experimented with double breaks in cooling pipes to provide data that could be used to help develop and assess the computer models." In some early experiments, the researchers put food coloring in the water to check where the cooling water went in an accident. The phrase "all the green water went on the floor" wasn't good but the experiments at Semiscale were and caused the Atomic Energy Commission to adopt more conservative licensing and operating requirements.

Larson adds, "Interestingly, the accident at Three Mile Island was a result of small break loss of coolant, not the large break LOCAs conducted at Semiscale. Luckily, the Loss Of Fluid Test facility at the Test Area North as well as the Semiscale facility could be modified and used and did conduct a series of small break LOCA experiments."

Nowadays Larson is involved with many scaling projects ranging from developing a nonintrusive flow device for Advanced Test Reactor applications to measuring the flow rate of cold air entering and warm air exiting manufactured homes. He has spent the last several months building support and establishing the groundwork for the new lab-wide computing initiative. But Larson is looking forward to the challenge of subsurface fate and transport research.

Roughly 1/1700th the size of a power reactor, the Semiscale facility was built to help understand what happens in a massive loss of coolant accident.

"Reactor scaling had enough nonlinearity but, at least as far as we know, it is primarily a single scale problem. Subsurface fate and transport is a multi-scale problem. Fluid-flow, radiation, porosity, biological effects, etc. all have to be considered. And there are extremes of scale - geological time scale covers epochs, other temporal scales will be much smaller and multiple physical scales exist. From a scaling viewpoint, researchers know they have a problem, they just don't know the magnitude."

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Artificial Intelligence - The property of a machine capable of reason by which it can learn functions normally associated with human intelligence.

Gail Cordes doesn't care for the popular term 'artificial intelligence.' She prefers the more accurate 'intelligent information processing' or 'computational intelligence.' Whatever the term used, it is the extraordinary concept of increasing computer efficiency by mimicking ways the human brain processes information.

Cordes has been involved with intelligent information processing since 1988 and describes it then as a "bootstrap operation." The program has gone far in the intervening years. She explained some of the applications that cross-organizational teams have developed at the INEEL.

Expert systems - computer systems composed of algorithms that execute specialized, usually difficult professional tasks - are designed to perform at the level of or even beyond the level of a human expert. Expert systems follow a series of logic steps, with each path defined by a 'yes-no' response.

Back in '88, Cordes was the project manager for the Nuclear Regulatory Commission's Reactor Safety Assessment System. This expert system used plant data to assess the safety status of a commercial nuclear power reactor experiencing a long-term disturbance. More recently, a team of researchers from Waste Management Technologies has developed a data review expert system that is employed in the passive/active neutron and gamma assay conducted at the Stored Waste Examination Pilot Plant (SWEPP) on the INEEL. The system analyzes data on the waste drums and flags discrepancies for a human to review.

Fuzzy logic is called the logic of approximate reasoning and deals with uncertainties. It allows for interpretation and 'decision-making' by computers and is now so accepted that common household appliances are advertised as having it. "Powerful but surprisingly simple" Cordes describes it. In one of Cordes' early successes using this tool, she and two colleagues from Industrial and Material Technologies demonstrated a fuzzy control system for the Cybertran, the electronic train developed at the INEEL.

A data review expert system is employed in the passive/active neutron and gamma assay conducted at SWEPP. The expert system flags discrepancies for a human to review.

Cordes' current projects are also team efforts, supported by funding and direction from programs outside of National Security. One project, through Waste Management Technologies, employs pattern recognition to monitor the performance of nondestructive assay technologies. NDA technologies are used to characterize materials and container contents and the resulting characterization information becomes an historic, archival record. The software program uses the patterns of historic operation data to evaluate the ongoing equipment operation, providing real-time capability to monitor and defend performance. This software is also being used to interpret the NDA characterization measurement data.

A layperson may call these techniques artificial intelligence but Cordes says that by whatever name you use, it can assist humans in everything from safely running a nuclear reactor to more accurately interpreting X-rays.

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